Toughness-Inducing Additive Atoms Localized

Unprecedented transmission electron microscopy studies performed with the new One-Ångstrom Microscope (OÅM) at the National Center for Electron Microscopy (NCEM) have shown that the observed doubling of the toughness of a silicon nitride ceramic as a result of the addition of small amounts of yttrium oxide can be traced to the localization of the yttrium atoms in amorphous layers in extended SiN grain boundaries. The result is of great importance for the understanding of interfacial bonding and consequently the fracture properties of ceramics.

The mechanical properties of ceramics are strongly influenced by their microstructure, especially the local atomic structure at their grain boundaries. High-resolution transmission electron microscopy (HRTEM) has been used for many years to investigate ceramic grain boundaries but it had not been possible to combine this atomic scale structure with chemical information regarding the identity of atoms. Recent advances in microscope design and image simulation and processing at NCEM have extended the resolution of HRTEM to the sub-Ångstrom level (MSD Highlight 99-9). At this resolution, both imaging and identification of single columns of atoms are possible.

In this work, investigators in MSD's Ceramic Science Program heat treated Si_3N_4 with 2wt% yttrium oxide. Exposure of the material to 1400°C for 100 hours led to a ~100% increase in toughness. Lattice images of the heat-treated material obtained with the OÅM were compared with calculated images from a model with yttrium atoms localized in the 0.5-0.7 nm thin films of amorphous glass that reside at the intergranular interfaces. The observed and simulated images agreed (see figure), indicating that the yttrium atoms segregate to specific sites at these boundaries.

The observed increased toughness was accompanied by a dramatic change in the fracture mechanism of the material from transgranular (through the grains) to intergranular (along the grain), a phenomenon thought to result from a weakening in the grain boundaries. Since intergranular cracking promotes "bridging" between the crack surfaces due to interlocking grains, this could explain the significantly enhanced toughness.

The results show that minute changes in atom location (i.e., addition of Y atoms to the grain boundaries) can have a large effect on the strength of grain boundaries and therefore a profound influence on the fracture toughness. They also demonstrate that the increased sensitivity of HRTEM that accompanies the resolution improvements and correction of lens aberrations is extremely valuable for fundamental investigations of the nanoscale amorphous intercrystalline films that determine many of the important properties of ceramics. The increased understanding of the precise composition of ceramic grain boundaries is critical to developing new and improved ceramic microstructures with superior structural performance.

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A. Ziegler, C. Kisielowski, and R.O. Ritchie, "Imaging of the crystal structure of silicon nitride at 0.8 Ångström resolution," *Acta Materialia* **50**, 565-574 (2002).